Dichloroacetylene

7572-29-4 | DTXSID7020429

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 68.5 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.98e-01

Confidence level: 7.49e-01

Nearest Neighbors from the Training Set

Image not found
Chloroform
Measured: 39.8
Predicted: 50.3

Image not found
Chloropicrin
Measured: 61.7
Predicted: 61.7

Image not found
Trichloroethylene
Measured: 100
Predicted: 83.1

Image not found
1,2-Dibromoethane
Measured: 51.3
Predicted: 55.8

Image not found
Carbon disulfide
Measured: 219
Predicted: 167